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Flow towards diagonalization for Many-Body-Localization models : adaptation of the Toda matrix differential flow to random quantum spin chains

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The iterative methods to diagonalize matrices and many-body Hamiltonians can be reformulated as flows of Hamiltonians towards diagonalization driven by unitary transformations that preserve the spectrum. After a comparative overview of the various types of discrete flows (Jacobi, QR-algorithm) and differential flows (Toda, Wegner, White) that have been introduced in the past, we focus on the random XXZ chain with random fields in order to determine the best closed flow within a given subspace of running Hamiltonians. For the special case of the free-fermion random XX chain with random fields, the flow coincides with the Toda differential flow for tridiagonal matrices which is related to the classical integrable Toda chain and which can be seen as the continuous analog of the discrete QR-algorithm. For the random XXZ chain with random fields that displays a Many-Body-Localization transition, the present differential flow should be an interesting alternative to compare with the discrete flow that has been proposed recently to study the Many-Body-Localization properties in a model of interacting fermions (L. Rademaker and M. Ortuno, Phys. Rev. Lett. 116, 010404 (2016)).

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I. INTRODUCTION

In the field of Many-Body Localization (see the recent reviews [1, 2] and references therein), the focus is on the unitary dynamics of isolated random interacting quantum systems, so that one needs to understand the properties of the whole set of excited eigenstates. It is thus interesting to revisit the methods that have been proposed to diagonalize matrices and many-body Hamiltonians.

Whenever the eigenstates are not obvious, it is natural to devise iterative strategies. For matrices, the idea to introduce an iterative method to converge towards diagonalization goes back to the algorithm of Jacobi in 1846 [3] : the principle is to use iteratively elementary two by two rotations in order to eliminate the corresponding off-diagonal terms. This procedure has been adapted to many-body second-quantized Hamiltonians by White [4] and has been applied recently to the problem of Many-Body Localization for interacting fermions by Rademaker and Ortuno [5]. Another possibility is to use continuous unitary transformations as proposed independently by Wegner for condensed matter models [6] (see the reviews [7], the book [8] and references therein), by Glazek and Wilson for high-energy models [9], and by mathematicians for optimization problems [10, 11] under the name "double bracket flow". In this continuous framework, various generators have been introduced : for instance the Wegner generator [6–8] eliminates more rapidly the off-diagonal terms corresponding to larger differences of the corresponding diagonal terms, while the White generator [4] eliminates all off-diagonal terms with the same exponential rate.

In all the schemes mentioned above, the goal is to obtain some systematic decrease of the off-diagonal part of the Hamiltonian. However, there exists a completely different strategy to converge towards diagonalization (see for instance the book [12] and references therein) : the "power method" consists in the successive applications $H^n|v_0>$ of the Hamiltonian H onto some initial vector $|v_0>$ to converge towards the eigenvector associated to the biggest eigenvalue; the successive applications of the Hamiltonian can actually be kept to build the Krylov subspace spanned by the successive vectors $(|v_0>, H|v_0>, ..., H^n|v_0>)$ and to construct its orthogonal basis via the Lanczos algorithm; finally, instead of applying H to a single vector, the Hamiltonian can be applied to a basis of vectors $(|v_i>)$ in order to obtain the new vectors $H|v_i>$ and to produce a new basis after orthonormalization : this is the so-called QR-algorithm. It turns out that the continuous formulation of this strategy displays very remarkable properties that have been much studied under the name of "Toda flow" for tridiagonal matrices (see for instance [13–21]) as a consequence of its relation to the classical integrable Toda lattice [22]. Note that exactly the same generator of continuous unitary transformations has been re-discovered independently by Mielke [23] via the requirement to obtain a closed flow for band matrices, i.e. to maintain the 'sparsity' of the initial matrix.

For Many-Body Hamiltonians, the idea to avoid that the diagonalization flow invades the whole space of possible running Hamiltonians is of course even more essential. The goal of the present paper is thus to try to adapt the strategy of Toda differential flow of tridiagonal matrices to random quantum spin chains. However since the literature on the various methods described above is scattered over various communities, with various ideas re-invented several times independently, it seems useful to give first some comparative overview of the different frameworks.

The paper is organized as follows. In Section II, the notion of flow towards diagonalization via unitary transformations is presented with its invariants, both for matrices and for Many-Body quantum spin chains. For matrices, discrete flows (Jacobi, QR) are described in Section III, while the continuous flows (Wegner, White, Toda) are recalled in Section IV. For random quantum spin chains, the discrete flow translated from the corresponding interacting fermions formulation (White, Rademaker-Ortuno) is presented in Section V, while the continuous framework is given in Section VI. In section VII, we adapt the idea of the Toda flow for the XXZ chain. Our conclusions are summarized in section VIII.

II. NOTION OF FLOW TOWARDS DIAGONALIZATION

The goal is to diagonalize the Hamiltonian H, i.e. to find the eigenvalues E_i and the corresponding eigenstates $|\psi_i>$

$$H = \sum_i E_i |\psi_i >< \psi_i| \tag{1}$$

via an iterative procedure based on unitary transformations.

A. Family of unitary transformations

Let l be an index that can be either discrete $l = 0, 1, 2, ..$ or continuous $l \in [0, +\infty[$. One wishes to construct a series of unitary transformation $U(l)$

$$U(l)U^\dagger(l) = U^\dagger(l)U(l) = 1 \tag{2}$$

so that the running Hamiltonian

$$H(l) = U(l)HU^\dagger(l) \tag{3}$$

starting at $H(l = 0) = H$ converges towards diagonalization as $l \to +\infty$. Note that this goal is very ambitious for complex models, since all information is kept along the flow, in contrast to renormalization methods that try to eliminate iteratively the irrelevant information.

B. Invariants of the flow

Since the flow built from unitary transformations conserves the eigenvalues E_i, it is interesting to construct the invariants corresponding to the traces of the integer powers of the Hamiltonian

$$I_p \equiv \sum_i E_i^p = \mathrm{Tr}(H^p(l)) \tag{4}$$

The conservation of the invariant for $p = 1$ leads to the sum rule of the diagonal elements $H_{n,n}(l)$ in terms of the energies E_i

$$I_1 \equiv \sum_i E_i = Tr(H(l)) = \sum_n H_{n,n}(l) \tag{5}$$

The conservation of the invariant for $p = 2$ leads to the sum rule for the square of the modulus of the matrix elements

$$I_2 \equiv \sum_i E_i^2 = Tr(H^2(l)) = \sum_n \sum_m H_{n,m}(l)H_{m,n}(l) = \sum_n \sum_m |H_{n,m}(l)|^2 \tag{6}$$

This means that its diagonal and off-diagonal contributions

$$\begin{aligned} I_2 &= I_2^{diag}(l) + I_2^{off}(l) \\ I_2^{diag}(l) &\equiv \sum_n H_{n,n}^2(l) \\ I_2^{off}(l) &\equiv \sum_n \sum_{m \neq n} |H_{n,m}(l)|^2 \end{aligned} \tag{7}$$

have opposite variations

$$\frac{dI_2^{diag}(l)}{dl} = -\frac{dI_2^{off}(l)}{dl} \tag{8}$$

The goal of full diagonalization at $l = +\infty$ corresponds to

$$\begin{aligned} I_2^{off}(l = +\infty) &= 0 \\ I_2^{diag}(l = +\infty) &= I_2 = \sum_i E_i^2 \end{aligned} \tag{9}$$

This second invariant allows to distinguish between two types of strategies :

(i) either one imposes that the off-diagonal contribution $I_2^{off}(l)$ is always decaying from its initial value $I_2^{off}(l = 0)$ towards its vanishing final value $I_2^{off}(l = +\infty) = 0$

$$\frac{dI_2^{off}(l)}{dl} < 0 \tag{10}$$

(ii) or the only condition imposed on the dynamics of off-diagonal contribution $I_2^{off}(l)$ is its final vanishing final value $I_2^{off}(l = +\infty) = 0$. To obtain this long-term objective, one is ready to accept a temporary increase of $I_2^{off}(l)$ along the flow.

C. Application to Many-Body Hamiltonians

For many-body Hamiltonians, one can consider that the Hamiltonian is represented by a matrix in a given basis of the Hilbert space and apply the methods developed for matrices. However it seems much more appropriate to define the diagonalization flow in terms of the coupling constants in front of second-quantized operators.

For instance for a chain of N quantum spins described by the the hermitian Pauli matrices at each site

$$\sigma^{(0)} = Id = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z \quad = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{11}$$

the most general running Hamiltonian for N spins can be expanded in the basis of Pauli matrices as

$$H(l) = \sum_{a_1=0,x,y,z} ... \sum_{a_N=0,x,y,z} H_{a_1...a_N}(l)\sigma_1^{(a_1)}\sigma_2^{(a_2)}...\sigma_N^{(a_N)} \tag{12}$$

with the 4^N real coefficients

$$H_{a_1...a_N}(l) = \frac{1}{2^N} Tr(H(l)\sigma_1^{(a_1)}\sigma_2^{(a_2)}...\sigma_N^{(a_N)}) \tag{13}$$

The diagonal part

$$H_{diag}(l) = \sum_{a_1=0,z} ... \sum_{a_N=0,z} H_{a_1...a_N}(l)\sigma_1^{(a_1)}\sigma_2^{(a_2)}...\sigma_N^{(a_N)} \tag{14}$$

involves the 2^N real coefficients $H_{a_1...a_N}(l)$, where each a_i takes only the two values $a_i = 0, z$. The goal is to flow towards this diagonal form, and thus to eliminate the off-diagonal part

$$H_{off}(l) = H(l) - H_{diag}(l) \tag{15}$$

that contains some Pauli matrices $\sigma_i^{a_i}$ with the values $a_i = x, y$.

Here it is convenient to normalize the invariants as

$$I_q = \frac{1}{2^N} Tr(H^q(l)) \tag{16}$$

The first invariant $q = 1$ given by the coefficient of Eq. 13 where all indices vanish $a_i = 0$

$$I_1 = \frac{1}{2^N} Tr(H(l)) = H_{0,0,0,..0}(l) \tag{17}$$

simply represents the middle of the spectrum and can be chosen to vanish.

The second invariant corresponds to the sum of the squares of all coefficients of Eq. 12

$$I_2 = \frac{1}{2^N} Tr(H^2(l)) = \sum_{a_1=0,x,y,z} ... \sum_{a_N=0,x,y,z} H^2_{a_1...a_N}(l) \tag{18}$$

with the diagonal and off-diagonal contributions

$$\begin{aligned} I_2^{diag}(l) &= \frac{1}{2^N} Tr(H^2_{diag}(l)) = \sum_{a_1=0,z} ... \sum_{a_N=0,z} H^2_{a_1...a_N}(l) \\ I_2^{off}(l) &= I_2 - I_2^{diag}(l) \end{aligned} \tag{19}$$

D. Example of the XXZ chain with random fields

The quantum spin chains with local interactions are of course extremely sparse with respect to the space of couplings of dimension 4^N discussed above. For instance, in the XXZ chain with random couplings and random fields, where the diagonal and off-diagonal parts read (the XX coupling is defined with respect to the ladder operators $\sigma^{\pm} = (\sigma^x \pm \sigma^y)/2$ for later convenience)

$$\begin{aligned} H^{XXZ}_{diag}(l=0) &= \sum_{i=1}^{N} (h_i \sigma_i^z + J_i^{zz} \sigma_i^z \sigma_{i+1}^z) \\ H^{XXZ}_{off}(l=0) &= \sum_{i=1}^{N} \frac{J_i}{2} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) = \sum_{i=1}^{N} J_i (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) \end{aligned} \tag{20}$$

the only non-vanishing coefficients of Eq. 13 are the N terms with only one non-vanishing index $a_i = z$, and the $(3N)$ terms with only two consecutive coinciding indices $a_i = a_{i+1} \neq 0$

$$H_{a_1...a_N}(l=0) = h_i \delta_{a_i,z} \prod_{j \neq i} \delta_{a_j,0} + J_i^{zz} \delta_{a_i,z} \delta_{a_{i+1},z} \prod_{j \neq (i,i+1)} \delta_{a_j,0} + \frac{J_i}{2} (\delta_{a_i,x} \delta_{a_{i+1},x} + \delta_{a_i,y} \delta_{a_{i+1},y}) \prod_{j \neq (i,i+1)} \delta_{a_j,0} \tag{21}$$

The first invariant of Eq. 17 vanishes while the second invariant of Eq. 19

$$\begin{aligned} I_2 &= I_2^{diag}(l=0) + I_2^{off}(l=0) \\ I_2^{diag}(l=0) &= \sum_i (h_i^2 + (J_i^{zz})^2) \\ I_2^{off}(l=0) &= \frac{1}{2} \sum_i J_i^2 \end{aligned} \tag{22}$$

grows linearly in N and fixes the variance of the Gaussian form of the density of states in the middle of the spectrum as in other local spin models [24, 25].

Via the standard Jordan-Wigner transformation onto anticommuting fermionic operators

$$\begin{aligned} c_i^\dagger &\equiv e^{i\pi \sum_{j=1}^{i-1} \sigma_j^+ \sigma_j^-} \sigma_i^+ \\ c_i &\equiv e^{-i\pi \sum_{j=1}^{i-1} \sigma_j^+ \sigma_j^-} \sigma_i^- \\ c_i^\dagger c_i &= \sigma_i^+ \sigma_i^- \end{aligned} \tag{23}$$

the XXZ Hamiltonian of Eq. 20 becomes

$$H^{XXZ}_{diag}(l=0) = \sum_{i=1}^{N} h_i (2c_i^\dagger c_i - 1) + \sum_{i=1}^{N} J_i^{zz} (2c_i^\dagger c_i - 1)(2c_{i+1}^\dagger c_{i+1} - 1) + \sum_{i=1}^{N} J_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) \tag{24}$$

The XX chain corresponding to $J^{zz} = 0$ is a free-fermion quadratic model that can be diagonalized into $H^{free} = \sum \epsilon_k f_k^\dagger f_k$ via a unitary transformation of the fermions operators from c_i to f_k, i.e. in the spin language, the diagonalization form obtained by the diagonalization flow at $l = +\infty$ should contain only N coefficients $h_i(l = +\infty)$

$$H^{XX}(l=+\infty) = \sum_{i=1}^{N} h_i(l=+\infty) \sigma_i^z \tag{25}$$

As a consequence, our first goal in this paper is to define a flow that remain sparse for the free-fermion XX chain between the sparse initial state of Eq. 20 and the sparse final state of Eq. 25.

For the XXZ chain with $J^{zz} \neq 0$, there exists a non-trivial density-density interaction in the fermion language of Eq. 24, so that one does not expect any simplification with respect to the most general diagonal form of Eq. 14 at $l = +\infty$

$$H^{XXZ}(l = +\infty) = \sum_{a_1=0,z} ... \sum_{a_N=0,z} H_{a_1...a_N}(l = +\infty)\sigma_1^{(a_1)}\sigma_2^{(a_2)}...\sigma_N^{(a_N)} \tag{26}$$

where the 2^N real coefficients are necessary to reproduce the 2^N eigenvalues. The form of Eq. 26 has been much discussed in the context of Many-Body Localization (see the recent reviews [1, 2] and references therein). In particular, in the Fully-Many-Body-Localized phase, the pseudo-spin operators at $l = +\infty$ that commute with each other and with the Hamiltonian are related to the initial spins by a *quasi-local* unitary transformation and the couplings $H_{a_1...a_N}(l = +\infty)$ decay exponentially with the distance with a sufficient rate so that there exists an extensive number of emergent *localized* conserved operators (see [5, 26–33] and the reviews [1, 2] for more details). In particular, these emergent conserved operators have a simple interpretation within the RSRG-X procedure that constructs the whole set of excited eigenstates [34–39] via the extension of the Strong Disorder Real-Space RG approach developed by Ma-Dasgupta-Hu [40] and Daniel Fisher [41, 42] to construct the ground states (see [43–45] for reviews). The Heisenberg chain in random fields h_i corresponding to the uniform couplings $J_i^{zz} = \frac{J_i}{2} = J$ is the model displaying a Many-Body-Localization transition that has been studied on the biggest sizes (see [46–48] and references therein).

For the XXZ chain, the final state of Eq. 26 thus contains 2^N coefficients, in contrast to the initial state containing only $4N$ coefficients (Eq 21). So here our goal will be to obtain a diagonalization flow $H_{XXZ}(l)$ that remain sparse with respect to the ladder operators.

III. DISCRETE DIAGONALIZATION FLOWS FOR MATRICES

A. Generator $\eta(l)$ associated to the elementary unitary transformations $u(l)$

When l is a discrete index, the unitary transformations $U(l)$ are constructed via some iteration

$$U(l) \equiv u(l)U(l-1) = u(l)u(l-1)u(l-2)...u(1) \tag{27}$$

in terms of elementary unitary transformations $u(l)$ that governs the flow of the running Hamiltonian of Eq. 3

$$H(l) = U(l)HU^\dagger(l) = u(l)H(l-1)u^\dagger(l) \tag{28}$$

It is convenient to introduce the anti-hermitian generator $\eta(l)$

$$\eta^\dagger(l) = -\eta(l) \tag{29}$$

associated to the elementary unitary transformations $u(l)$

$$u(l) \equiv e^{\eta(l)} \tag{30}$$

B. Jacobi's algorithm for matrices

In Jacobi's algorithm [3], one identifies the off-diagonal element with the biggest modulus of the matrix $H(l-1)$

$$|H_{mn}(l-1)| = \max_{i<j} |H_{ij}(l-1)| \tag{31}$$

The antihermitian generator of Eq. 32 is chosen as

$$\eta(l) = \theta_l e^{i\phi_l} |n><m| - \theta_l |m><n| \tag{32}$$

in order to produce the complex unitary rotation

$$u(l) \quad = e^{\eta(l)} = 1 + (\cos\theta_l - 1)(|m><m| + |n><n|) + \sin\theta_l (e^{i\phi_l}|n><m| - e^{-i\phi_l}|m><n|) \tag{33}$$

acting in the two-dimensional subspace (m, n) as

$$\begin{aligned} u(l)|m> &= \cos\theta_l|m> + e^{i\phi_l}\sin\theta_l|n> \\ u(l)|n> &= -e^{-i\phi_l}\sin\theta_l|m> + \cos\theta_l|n> \end{aligned} \tag{34}$$

The two angles θ_l and ϕ_l are chosen to make the off-diagonal element of $H(l)$ between m and n vanish

$$0 = H_{mn}(l) =< m|u(l)H(l-1)u^\dagger(l)|n> \tag{35}$$

yielding

$$0 = \cos^2\theta_l e^{i\phi_l} H^*_{nm}(l-1) - \sin^2\theta_l e^{-i\phi_l} H_{nm}(l-1) + \cos\theta_l\sin\theta_l\left(H_{mm}(l-1) - H_{nn}(l-1)\right) \tag{36}$$

The phase $e^{i\phi_l}$ is thus the phase of the off-diagonal element $H_{nm}(l-1)$

$$e^{i\phi_l} = \frac{H_{nm}(l-1)}{|H_{nm}(l-1)|} \tag{37}$$

while the remaining real equation for the angle θ_l

$$0 = \cos(2\theta_l)|H_{nm}(l-1)| + \sin(2\theta_l)\left(\frac{H_{mm}(l-1) - H_{nn}(l-1)}{2}\right) \tag{38}$$

is determined by the ratio between the off-diagonal element modulus and the difference between the diagonal elements

$$\begin{aligned} \tan(2\theta_l) &= \frac{2|H_{nm}(l-1)|}{H_{nn}(l-1) - H_{mm}(l-1)} \\ \cos(2\theta_l) &= \frac{1}{\sqrt{1+\tan^2(2\theta_l)}} \\ \sin(2\theta_l) &= \frac{\tan(2\theta_l)}{\sqrt{1+\tan^2(2\theta_l)}} \end{aligned} \tag{39}$$

The new diagonal elements correspond to the standard formula for the diagonalization of 2×2 matrices

$$\begin{aligned} H_{mm}(l) &= \frac{H_{mm}(l-1)+H_{nn}(l-1)}{2} + \frac{H_{mm}(l-1)-H_{nn}(l-1)}{2}\sqrt{1+\left(\frac{2|H_{nm}(l-1)|}{H_{nn}(l-1)-H_{mm}(l-1)}\right)^2} \\ H_{nn}(l) &= \frac{H_{nn}(l-1)+H_{mm}(l-1)}{2} + \frac{H_{nn}(l-1)-H_{mm}(l-1)}{2}\sqrt{1+\left(\frac{2|H_{nm}(l-1)|}{H_{nn}(l-1)-H_{mm}(l-1)}\right)^2} \end{aligned} \tag{40}$$

The sum is conserved as it should (Eq. 5)

$$I_1(l) - I_1(l-1) = H_{mm}(l) + H_{nn}(l) - H_{mm}(l-1) - H_{nn}(l-1) = 0 \tag{41}$$

while the diagonal contribution to the second invariant of Eq. 7 evolves according to

$$\begin{aligned} &I_2^{diag}(l) - I_2^{diag}(l-1) = H^2_{mm}(l) + H^2_{nn}(l) - H^2_{mm}(l-1) - H^2_{nn}(l-1) \\ &= (H_{mm}(l)+H_{nn}(l))^2 - (H^2_{mm}(l-1)+H^2_{nn}(l-1))^2 - 2H_{mm}(l)H_{nn}(l) + 2H_{mm}(l-1)H_{nn}(l-1) \\ &= 2H_{mm}(l-1)H_{nn}(l-1) - 2H_{mm}(l)H_{nn}(l) \\ &= 2|H_{nm}(l-1)|^2 \end{aligned} \tag{42}$$

So the maximum rule of Eq. 31 corresponds to the maximal growth of the diagonal contribution, and thus to the maximal decay of the off-diagonal contribution (Eq. 7) among the choice of elementary 2×2 rotations. Note however that the choice of the maximal off-diagonal element in Eq. 31 is not mandatory : one can choose a different order among the off-diagonal elements if it is more convenient for practical reasons, and the convergence towards diagonalization will be still ensured by Eq. 42.

C. QR algorithm for matrices

In the Jacobi algorithm described above, the goal is to obtain the systematic decrease of the off-diagonal part of the Hamiltonian. However there exist completely different strategies to converge towards diagonalization (see for instance the book [12] and references therein). For instance, the converge towards the eigenvector associated with the biggest eigenvalue can be achieved by the successive applications $H^n|v_0>$ of the Hamiltonian H onto some initial vector $|v_0>$, this is the so-called "power method". To obtain more eigenvectors, the successive applications of the Hamiltonian can be kept to build the Krylov subspace spanned by the successive iterations $(|v_0>, H|v_0>, ..., H^n|v_0>)$ and one orthogonal basis can be constructed via the Lanczos algorithm. When the goal is the full diagonalization, these ideas can be used slightly differently to obtain the so-called QR-algorithm : instead of applying H to a single vector, the Hamiltonian can be applied to the current basis $|i>$ of vectors to obtain the new vectors $H|i>$ in order to produce a new basis after orthonormalization : this amounts to the so-called QR-decomposition of the current Hamiltonian $H(l)$ into

$$H(l) = Q(l)R(l) \tag{43}$$

where $Q(l)$ is the orthogonal matrix ($Q(l)Q^t(l) = Id$) describing the change of bases and where $R(l)$ is the upper triangular matrix produced by the orthonormalization process of the vectors $(H|i>)$ (for instance via the Gram-Schmidt procedure or via the Householder reflections method). Then the writing of the Hamiltonian in the new basis gives the iteration

$$H(l+1) = Q^t(l)H(l)Q(l) = Q^t(l)(Q(l)R(l))Q(l) = R(l)Q(l) \tag{44}$$

This defines the QR-algorithm that converges towards diagonalization.

In summary, the QR-algorithm is an important example of a strategy not driven by the systematic decay of the off-diagonal elements via I_2^{off}, but based instead on the long-term expectation that the successive applications of the Hamiltonian will converge towards diagonalization asymptotically.

IV. CONTINUOUS DIAGONALIZATION FLOWS FOR MATRICES

A. Generator $\eta(l)$ of the infinitesimal unitary transformation

When the family of unitary transformation $U(l)$ is parametrized by a continuous parameter $l \in [0, +\infty[$, the elementary unitary transformation to go from l to $(l + dl)$ has some infinitesimal amplitude (dl) in front of the anti-Hermitian generator $\eta(l)$

$$U(l+dl) \quad = e^{dl\eta(l)}U(l) = U(l) + dl\eta(l)U(l) \tag{45}$$

Then the running Hamiltonian $H(l)$ evolves according to

$$H(l+dl) = e^{dl\eta(l)}H(l)e^{-dl\eta(l)} = H(l) + dl(\eta(l)H(l) - H(l)\eta(l)) \tag{46}$$

i.e. it satisfies the differential equation involving the commutator with the generator

$$\frac{dH(l)}{dl} = [\eta(l), H(l)] \tag{47}$$

In terms of the matrix elements of the anti-hermitian generator

$$\eta_{nk}(l) \quad = -\eta^*_{k,n}(l) \tag{48}$$

the off-diagonal matrix elements $n \neq q$ evolve according to

$$\frac{dH_{nq}(l)}{dl} \quad = -(H_{nn}(l) - H_{qq}(l))\eta_{nq}(l) + \sum_{k\neq(n,q)} (\eta_{nk}(l)H_{kq}(l) - H_{nk}(l)\eta_{kq}(l)) \tag{49}$$

while the evolution of the diagonal elements reads

$$\frac{dH_{nn}(l)}{dl} \quad = \sum_{k\neq n} (\eta_{nk}(l)H_{kn}(l) + \eta^*_{nk}(l)H^*_{kn}(l)) \tag{50}$$

The flow of the off-diagonal contribution $I_2^{off}(l)$ and of the diagonal contribution $I_2^{diag}(l)$ of Eq. 7 becomes

$$-\frac{dI_2^{off}(l)}{dl} = \frac{dI_2^{diag}(l)}{dl} = 2\sum_n H_{nn}(l)\frac{dH_{nn}(l)}{dl} = \sum_{n\neq k}(H_{nn}(l)-H_{kk}(l))\left(\eta_{nk}(l)H_{kn}(l)+\eta^*_{nk}(l)H^*_{kn}(l)\right) \tag{51}$$

B. Flows based on the systematic decay of $I_2^{off}(l)$

Generators of the form

$$\eta_{nk} = H_{nk}f(H_{nn}-H_{kk}) \tag{52}$$

where the function $f(x)$ is antisymmetric $f(x) = -f(-x)$ to insure the the antihermitian condition of Eq. 48 and satisfies $xf(x) \geq 0$ will produce flows with a systematic decay of $I_2^{off}(l)$ (Eq. 51)

$$0 < -\frac{dI_2^{off}(l)}{dl} = \frac{dI_2^{diag}(l)}{dl} = 2\sum_{n\neq k}|H_{nk}(l)|^2(H_{nn}(l)-H_{kk}(l))f(H_{nn}(l)-H_{kk}(l)) \tag{53}$$

1. *Wegner's choice $f^{Wegner}(x) = x$*

Wegner [6–8] has proposed to choose as generator

$$\eta^{Wegner}_{nk}(l) = H_{nk}(l)(H_{nn}(l)-H_{kk}(l)) \tag{54}$$

As the level of operators, these matrix elements correspond to the commutator between the diagonal part and the off-diagonal part of the Hamiltonian

$$\eta^{Wegner}(l) = [H_{diag}(l), H(l)] = [H_{diag}(l), H_{off}(l)] \tag{55}$$

Then $I_2^{off}(l)$ is a decreasing function (Eq. 51)

$$0 < -\frac{dI_2^{off}(l)}{dl} = \frac{dI_2^{diag}(l)}{dl} = \sum_{n\neq k}(H_{nn}(l)-H_{kk}(l))^2|H_{nk}|^2 \tag{56}$$

The off-diagonal matrix elements $n \neq q$ (Eq 49)

$$\frac{dH_{nq}(l)}{dl} = -(H_{nn}(l)-H_{qq}(l))^2H_{nq}(l) + \sum_{k\neq(n,q)} H_{nk}(l)H_{kq}(l)\big(H_{nn}(l)+H_{qq}(l)-2H_{kk}(l)\big) \tag{57}$$

are suppressed more rapidly when they are associated to large differences of diagonal elements $(H_{nn}(l) - H_{qq}(l))^2$. The equations of motion for the diagonal elements (Eq. 50)

$$\frac{dH_{nn}(l)}{dl} = 2\sum_{k\neq n}|H_{nk}(l)|^2(H_{nn}(l)-H_{kk}(l)) \tag{58}$$

and for the off-diagonal elements of Eq. 57 are polynomial of degree 3 in the matrix elements.

2. *White's choice $f^{White}(x) = \frac{1}{x}$*

White has proposed the generator (Eq. 18 of Reference [4])

$$\eta^{White}_{nk}(l) = \frac{H_{nk}(l)}{H_{nn}(l)-H_{kk}(l)} \tag{59}$$

Then the dynamics of $I_2^{off}(l)$ (Eq. 51)

$$0 < -\frac{dI_2^{off}(l)}{dl} = 2\sum_{n\neq k} |H_{kn}(l)|^2 = 2I_2^{off}(l) \tag{60}$$

has the nice property to display the explicit exponential decay

$$I_2^{off}(l) = I_2^{off}(l=0)e^{-2l} \tag{61}$$

(The particular value 2 of the exponential decay e^{-2l} has no particular meaning and can be changed by a redefinition of the flow parameter l).

The choice of Eq. 59 can be seen as the infinitesimal counterpart of the Jacobi choice of Eq. 39 and of the convergence rate towards diagonalization of Eq. 42 : the difference is that instead of doing a single finite elementary rotation to eliminate the biggest off-diagonal element, one uses the commutativity of all infinitesimal rotations to make all the off-diagonal elements decay with the same rate.

The corresponding equations of motion for the off-diagonal matrix elements $n \neq q$ (Eq 49)

$$\frac{dH_{nq}(l)}{dl} = -H_{nq}(l) + \sum_{k\neq(n,q)} H_{nk}(l)H_{kq}(l)\left(\frac{1}{H_{nn}(l)-H_{kk}(l)} - \frac{1}{H_{kk}(l)-H_{qq}(l)}\right) \tag{62}$$

and for the diagonal elements (Eq. 50)

$$\frac{dH_{nn}(l)}{dl} = 2\sum_{k\neq n} \frac{|H_{nk}(l)|^2}{H_{nn}(l)-H_{kk}(l)} \tag{63}$$

now contain denominators involving differences of diagonal elements that are usual in perturbation theory.

This direct link with perturbation theory can be clarified as follows. If one decomposes the generator η according to the order with respect to off-diagonal elements

$$\eta = \eta^{(1)} + \eta^{(2)} + \eta^{(3)} + ... \tag{64}$$

the dynamics reads

$$\begin{aligned}\frac{dH(l)}{dl} &= [\eta^{(1)} + \eta^{(2)} + \eta^{(3)} + ..., H_{diag} + H_{off}] \\ &= [\eta^{(1)}, H_{diag}] + \Big([\eta^{(1)}, H_{off}] + [\eta^{(2)}, H_{diag}]\Big) + \Big([\eta^{(2)}, H_{off}] + [\eta^{(3)}, H_{diag}]\Big) + ..\end{aligned} \tag{65}$$

White's choice written in Eq. 59 for matrix elements can be translated at the level of operators into the requirement

$$[\eta^{White}, H_{diag}] = -H_{off} \tag{66}$$

for the first term in the expansion of Eq. 65, in order to produce the exponential decay for the whole operator H_{off} (i.e. the same exponential decay for all off-diagonal matrix elements as given by the first term of Eq. 62). The form of Eq. 66 to determine the generator of unitary transformation corresponds to the Schrieffer-Wolff transformations at first order in perturbation theory (see the review [49]) that have been much used recently for random quantum spin chains to derive renormalization rules for the ground state [50] or for excited states in the Many-Body Localized Phase [34, 38].

3. Intermediate sign choice $f^{sgn}(x) = \text{sgn}(x)$

As an intermediate between the previous Wegner's and White's proposals, the sign choice [52]

$$\eta_{nk}^{sign}(l) = H_{nk}(l)\text{sgn}(H_{nn}(l) - H_{kk}(l)) \tag{67}$$

corresponds to the convergence criterion

$$0 < -\frac{dI_2^{off}(l)}{dl} = \frac{dI_2^{diag}(l)}{dl} = 2\sum_{n\neq k} |H_{nn}(l) - H_{kk}(l)||H_{nk}(l)|^2 \tag{68}$$

and to the flow equations for the off-diagonal elements

$$\frac{dH_{nq}(l)}{dl} = -|H_{nn}(l) - H_{qq}(l)|H_{nq}(l) + \sum_{k\neq(n,q)} H_{nk}(l)H_{kq}(l)\big(\mathrm{sgn}(H_{nn}(l) - H_{kk}(l)) + \mathrm{sgn}(H_{qq}(l) - H_{kk}(l))\big) \tag{69}$$

and the diagonal elements

$$\frac{dH_{nn}(l)}{dl} = 2\sum_{k\neq n} |H_{nk}(l)|^2 \mathrm{sgn}(H_{nn}(l) - H_{kk}(l)) \tag{70}$$

4. *Comparison of the phase space contraction*

To simplify the discussion, let us focus on the case where H is a real symmetric matrix : there are M diagonal matrix elements H_{nn} with $n = 1, .., M$ and $\frac{M^2-M}{2}$ off-diagonal matrix elements H_{nq} with $1 \leq n < q \leq M$.

Then the dynamical equations for the matrix elements are of the form

$$\frac{dH_{n\leq q}(l)}{dl} = V_{nq}(H(l)) \tag{71}$$

in terms of the velocity field

$$\begin{aligned} V_{n<q}(H) &= -H_{nq}(H_{nn} - H_{qq})f(H_{nn} - H_{qq}) \\ &+ \sum_{k\neq(n,q)} \left[\theta_{k<n}H_{kn} + \theta_{n<k}H_{nk}\right]\left[\theta_{k<q}H_{kq} + \theta_{q<k}H_{qk}\right](f(H_{nn} - H_{kk}) + f(H_{qq} - H_{kk})) \end{aligned} \tag{72}$$

and

$$V_{nn}(H) = 2\sum_{k\neq n} \left[\theta_{k<n}H_{kn}^2 + \theta_{n<k}H_{nk}^2\right] f(H_{nn} - H_{kk}) \tag{73}$$

where $\theta_{k<n} = 1$ if $k < n$ and zero otherwise.

If the initial condition is described by some probability distribution $\rho_{l=0}(H)$ with the elementary volume element

$$d\mathcal{V} \equiv \prod_{n=1}^{M} dH_{nn} \prod_{1\leq n<q\leq M} dH_{ij} \tag{74}$$

the dynamics is governed by the continuity equation

$$\frac{\partial\rho_l(H)}{\partial l} = -\vec{\nabla}.\left[\rho_l(H)\vec{V}\right] = -\rho_l(H)\left[\vec{\nabla}.\vec{V}\right] - \vec{V}.\vec{\nabla}\rho_l(H) \tag{75}$$

where the first term containing the divergence of the velocity field $\left[\vec{\nabla}.\vec{V}\right]$ represents the contraction of the phase space volume of Eq. 74, while the second term contains the advective derivative $\vec{V}.\vec{\nabla}$ familiar from hydrodynamics.

While the off-diagonal directions are always contracting

$$\frac{\partial V_{n<q}}{\partial H_{n<q}} = -(H_{nn} - H_{qq})f(H_{nn} - H_{qq}) < 0 \tag{76}$$

the diagonal directions correspond to contraction if $f'(x) < 0$ or to expansion if $f'(x) > 0$.

$$\frac{\partial V_{nn}}{\partial H_{nn}} = 2\sum_{k\neq n} H_{kn}^2 f'(H_{nn} - H_{kk}) \tag{77}$$

As a consequence, the global resulting divergence of the velocity field

$$\begin{aligned} \vec{\nabla}.\vec{V} &= \sum_{1\leq n\leq M} \frac{\partial V_{nn}}{\partial H_{nn}} + \sum_{1\leq n<q\leq M} \frac{\partial V_{n<q}}{\partial H_{n<q}} \\ &= 4\sum_{1\leq n<q\leq M} H_{nq}^2 f'(H_{nn} - H_{qq}) - \sum_{1\leq n<q\leq M} (H_{nn} - H_{qq})f(H_{nn} - H_{qq}) \end{aligned} \tag{78}$$

depends on the choice of the function f. For the three cases described above

$$\begin{aligned}
\frac{df^{Wegner}}{dx} &= 1 \geq 0 \\
\frac{df^{White}}{dx} &= -\frac{1}{x^2} \leq 0 \\
\frac{df^{sgn}}{dx} &= 2\delta(x) = 0 \quad \text{for} \quad x \neq 0
\end{aligned} \tag{79}$$

one obtains the corresponding divergences

$$\vec{\nabla}.\vec{V}^{Wegner} = 4 \sum_{1\leq n<q\leq M} H_{nq}^2 - \sum_{1\leq n<q\leq M} (H_{nn} - H_{qq})^2 \tag{80}$$

$$\vec{\nabla}.\vec{V}^{White} = -4 \sum_{1\leq n<q\leq M} \frac{H_{nq}^2}{(H_{nn} - H_{qq})^2} - \sum_{1\leq n<q\leq M} 1 \tag{81}$$

$$\vec{\nabla}.\vec{V}^{sgn} = 8 \sum_{1\leq n<q\leq M} H_{nq}^2 \delta(H_{nn} - H_{qq}) - \sum_{1\leq n<q\leq M} |H_{nn} - H_{qq}| \tag{82}$$

So while the White's flow and the sign flow are always contracting, Wegner's flow can be expanding in the initial stage as long as the off-diagonal part has not decreased sufficiently.

C. Toda flow

In the above continuous flows based on the systematic decay of I_2^{off} ensured by generators of the form of Eq. 52, it is impossible to avoid the generation of new matrix elements even if the initial condition is sparse. It is thus interesting to look for other flows that can preserve the sparsity of the initial matrix.

1. *Closed flow for band matrices*

If the initial matrix has some band structure

$$H_{nk}(l = 0) = 0 \quad \text{for} \quad |n - k| > B \tag{83}$$

it is possible to preserve this structure via the flow if one chooses the generator

$$\eta_{nk}^{Toda} = H_{nk}\text{sgn}(k - n) \tag{84}$$

because the flow equation for the off-diagonal terms read

$$\frac{dH_{nq}}{dl} = -(H_{nn} - H_{qq})H_{nq}\text{sgn}(q - n) + \sum_{k\neq(n,q)} H_{nk}H_{kq} \left(\text{sgn}(k - n) + \text{sgn}(k - q)\right) \tag{85}$$

while the diagonal terms evolve according to

$$\frac{dH_{nn}}{dl} = 2\sum_{k\neq n} |H_{nk}|^2 \text{sgn}(k - n) \tag{86}$$

The generator of Eq. 84 has been re-discovered by Mielke [23] from the requirement to obtain a closed flow for band matrices, but has actually a long history for the special case of real tridiagonal matrices as we now recall.

2. *Toda flow for tridiagonal real matrices*

For the special case of tridiagonal real matrices, where the only non-vanishing elements are the diagonal elements H_{nn} and the off-diagonal elements $H_{n,n+1} = H_{n+1,n}$, the closed flow based on the generator of Eq. 84

$$\begin{aligned}
\frac{dH_{nn}}{dl} &= 2(H_{n,n+1}^2 - H_{n-1,n}^2) \\
\frac{dH_{n,n+1}}{dl} &= H_{n,n+1}(H_{n+1,n+1} - H_{nn})
\end{aligned} \tag{87}$$

have been much studied under the name of "Toda flow" [13–21] as a consequence of its relation to the classical integrable Toda lattice [22] via a change of variables : the essential idea is that the flow equation of Eq. 47 corresponds to a Lax Pair equation for the integrable Toda model.

3. *Convergence towards diagonalization*

For our present perspective, the most important result is that this Toda flow converges towards diagonalization as first proven by Moser [15]

$$H_{n,n+1}(l=\infty)=0 \tag{88}$$

with ordered eigenvalues

$$H_{11}(\infty)>...>H_{NN}(\infty) \tag{89}$$

This result can be understood at the level of the differential equations by rewriting the flow of the diagonal terms (Eq. 87) as

$$\begin{aligned}
\frac{dH_{11}}{dl} &= 2H_{1,2}^2 \geq 0 \\
\frac{dH_{11}}{dl}+\frac{dH_{22}}{dl} &= 2H_{2,3}^2 \geq 0 \\
\frac{dH_{11}}{dl}+\frac{dH_{22}}{dl}+\frac{dH_{33}}{dl} &= 2H_{3,4}^2 \geq 0 \\
... \\
\sum_{n=1}^{N-1}\frac{dH_{nn}}{dl} &= 2H_{N-1,N}^2 \geq 0
\end{aligned} \tag{90}$$

so that $H_{11}(l)$, $(H_{11}(l)+H_{22}(l))$, etc are non-decreasing functions. Since they are bounded as a consequence of the invariants of the flow, they have to converge towards finite values $H_{nn}(l=+\infty)$ at $l=+\infty$. So the off-diagonal elements $H_{n,n+1}(l)$ representing their derivatives (Eq. 90) have to vanish $H_{n,n+1}(l=\infty)=0$ at $l=+\infty$. The flow of the off-diagonal element $H_{n,n+1}$ (Eq 87) can converge towards zero only if the corresponding diagonal elements satisfy the order $H_{nn}(l)>H_{n+1,n+1}(l)$ asymptotically for large l.

4. *Interpretation as some continuous limit of the QR-algorithm*

To understand the physical meaning of the Toda flow, it is important to stress that it can be interpreted as some continuous limit of the QR-algorithm recalled in section III C as follows. From the current orthonormal basis $|i_t>$ with $i=1,..,N$, one constructs the N infinitesimally-different vectors by the application of the Hamiltonian :

$$|v_{i_t}>=(1+dtH)|i_t>=|i_t>(1+dt<i_t|H|i_t>)+\sum_{j\neq i}|j_t>(dt<j_t|H|i_t>) \tag{91}$$

Now one needs to orthonormalize them to obtain a new basis. The Gram-Schmidt procedure begins with the normalization of the first vector $i=1$. Using

$$<v_{1_t}|v_{1_t}>=(1+2dt<i_t|H|i_t>) \tag{92}$$

one obtains the first normalized vector of the new basis as

$$|1_{t+dt}>=\frac{|v_{1_t}>}{\sqrt{<v_{1_t}|v_{1_t}>}}=|1_t>+\sum_{j>1}|j_t>(dt<j_t|H|1_t>) \tag{93}$$

Then the second vector $|v_{2_t}>$ is made orthogonal to the previous vector of Eq. 93 via the computation of the scalar product

$$<1_{t+dt}|v_{2_t}>=dt(<1_t|H|2_t>+<2_t|H|1_t>) \tag{94}$$

and the construction of

$$\begin{aligned} |w_{2_t}> &= |v_{2_t}> - |1_{t+dt}>< 1_{t+dt}|v_{2_t}> \\ &= |2_t> (1 + dt < 2_t|H|2_t>) - |1_t> (dt < 2_t|H|1_t>) + \sum_{j>2} |j_t> (dt < j_t|H|2_t>) \end{aligned} \tag{95}$$

and its normalization to obtain the second vector of the new basis

$$|2_{t+dt}>= \frac{|w_{2_t}>}{\sqrt{< w_{2_t}|w_{2_t}>}} = |2_t> - |1_t> (dt < 2_t|H|1_t>) + \sum_{j>2} |j_t> (dt < j_t|H|2_t>) \tag{96}$$

So one sees that the sign function in the Toda generator directly comes from this orthonornmalization procedure. Similarly by iteration one obtains all vectors of the new basis as

$$|i_{t+dt}>= |i_t> - \sum_{j<i} |j_t> (dt < i_t|H|j_t>) + \sum_{j>i} |j_t> (dt < j_t|H|2_t>) \tag{97}$$

that corresponds exactly to the Toda generator of Eq. 84.

More discussions on relations between the Toda flow and the QR algorithm can be found in Refs [16–21], together with the correspondences between other differential flows and other discrete matrix algorithms. In particular, one important output of these studies [16–18] is the formal solution of the Toda flow for the running Hamiltonian $H(l)$ in terms of the initial Hamiltonian $H(0)$

$$H(l) = Q^t(l)H(0)Q(l) \tag{98}$$

where the orthogonal matrix $Q(l)$ is the orthogonal matrix appearing in the QR-decomposition (where $R(l)$ is upper-triangular as in section III C) of the operator

$$e^{tH(0)} = Q(l)R(l) \tag{99}$$

To this give a clear physical meaning of the Toda flow.

V. DISCRETE FRAMEWORK FOR QUANTUM SPIN HAMILTONIANS

A. Expansion of the off-diagonal parts with ladder operators

In the expansion of the running Hamiltonian of Eq. 12 in terms of Pauli matrices, it is convenient to replace the off-diagonal Pauli matrices (σ^x, σ^y) by the the linear combinations corresponding to the ladder operators

$$\begin{aligned} \sigma^+ &= \frac{\sigma^x + i\sigma^y}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \sigma^- &= \frac{\sigma^x - i\sigma^y}{2} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{aligned} \tag{100}$$

because they are nilpotent

$$\begin{aligned} (\sigma^+)^2 &= 0 \\ (\sigma^-)^2 &= 0 \end{aligned} \tag{101}$$

and their products correspond to projectors π^{σ^z}

$$\begin{aligned} \sigma^+\sigma^- &= \frac{1 + \sigma^z}{2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \equiv \pi^+ \\ \sigma^-\sigma^+ &= \frac{1 - \sigma^z}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \equiv \pi^- \end{aligned} \tag{102}$$

The operator containing q_+ operators σ^+ on sites $1 \leq n_1 < n_2 < .. < n_{q_+} \leq N$, q_- operators σ^+ on different sites $1 \leq m_1 < m_2 < .. < m_{q_-} \leq N$ and $q_z \geq 0$ operators σ^z on further different sites $1 \leq p_1 < p_2 < .. < p_{q_z} \leq N$

$$X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} \equiv \sigma^z_{p_1}\sigma^z_{p_2}...\sigma^z_{p_{q_z}}\sigma^+_{n_1}\sigma^+_{n_2}...\sigma^+_{n_{q_+}}\ \sigma^-_{m_1}\sigma^-_{m_2}...\sigma^-_{m_{q_-}} \tag{103}$$

and its adjoint

$$X_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} \quad = \sigma^z_{p_1}\sigma^z_{p_2}...\sigma^z_{p_{q_z}}\sigma^-_{n_1}\sigma^-_{n_2}...\sigma^-_{n_{q_+}}\ \sigma^+_{m_1}\sigma^+_{m_2}...\sigma^+_{m_{q_-}} \tag{104}$$

are also nilpotent ($(X^\dagger)^2 = 0 = X^2 = 0$) and are associated to the projectors (Eq. 102)

$$\begin{aligned}
X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} X_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} &= \pi^+_{n_1}\pi^+_{n_2}...\pi^+_{n_{q_+}}\ \pi^-_{m_1}\pi^-_{m_2}...\pi^-_{m_{q_-}} \\
X_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} &= \pi^-_{n_1}\pi^-_{n_2}...\pi^-_{n_{q_+}}\ \pi^+_{m_1}\pi^+_{m_2}...\pi^+_{m_{q_-}}
\end{aligned} \tag{105}$$

The off-diagonal Hamiltonian can be decomposed as a sum over such operators

$$\begin{aligned}
H_{off}(l) = & \sum_{q_+=1}^{N} \sum_{q_-=0}^{N-q_+} \sum_{q_z=0}^{N-q_+-q_-} \sum_{n_{(1\leq\alpha\leq q_+)}} \sum_{m_{(1\leq\beta\leq q_-)}} \sum_{p_{(1\leq\alpha\leq q_z)}} \\
& \left[K_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} + K^*_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}}\right]
\end{aligned} \tag{106}$$

where the couplings can be obtained as

$$K_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) = 2^{q_++q_--N} Tr\left(X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} H(l)\right) \tag{107}$$

B. Adaptation of the Jacobi algorithm to quantum spin chains

The adaptation of the Jacobi diagonalization algorithm for matrices (recalled in section III B) to many-body second-quantized Hamiltonians has been introduced by White [4] and has been applied recently to the problem of Many-Body Localization for interacting fermions by Rademaker and Ortuno [5]. In the language of spin chains, the procedure can be summarized as follows. To suppress a given term

$$K_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} + J^*_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} \tag{108}$$

from the off-diagonal Hamiltonian of Eq. 106, one needs to consider the generalized unitary rotation of the form [5]

$$\begin{aligned}
u = e^{\eta} = \quad & e^{\theta\left(e^{i\phi}X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} - e^{-i\phi}X_{p_1,..p_{q_z}n_1,..,n_{q_+},m_1,..,m_{q_-}}\right)} \\
& = 1 + (\cos\theta - 1)(X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} \\
& \qquad + X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}}) \\
& + \sin\theta(e^{i\phi}X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} - e^{-i\phi}X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}})
\end{aligned} \tag{109}$$

where the angles (θ, ϕ) have to be chosen to obtain that the transformed coupling of Eq. 107 vanishes

$$\begin{aligned}
0 \quad & = K^{new}_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} = 2^{q_++q_--N} Tr\left(X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}}(uHu^\dagger)\right) \\
& = 2^{q_++q_--N} Tr\left(u^\dagger X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} uH\right)
\end{aligned} \tag{110}$$

Using the transformation of the operator X

$$\begin{aligned}
u^\dagger X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} u = & \cos^2\theta X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} - \sin^2\theta e^{i2\phi} X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} \\
& - \cos\theta\sin\theta e^{i\phi}(X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} \\
& \qquad - X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}})
\end{aligned} \tag{111}$$

Eq 110 becomes

$$\begin{aligned}
0 \quad & = K^{new}_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}} \\
& = \cos^2\theta K_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} - \sin^2\theta e^{i2\phi} K^*_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} \\
& - \cos\theta\sin\theta e^{i\phi} 2^{q_++q_--N} Tr\left(\left[\pi^+_{n_1}...\pi^+_{n_{q_+}}\ \pi^-_{m_1}...\pi^-_{m_{q_-}} - \pi^-_{n_1}...\pi^-_{n_{q_+}}\ \pi^+_{m_1}...\pi^+_{m_{q_-}}\right] H_{diag}\right)
\end{aligned} \tag{112}$$

So the angle ϕ has to be chosen as the phase of the coupling (analog to Eq. 37)

$$e^{i\phi} = \frac{K_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}}{|K_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}|} \tag{113}$$

and the angle θ has to be chosen as (analog to Eq. 39)

$$\tan(2\theta) = \frac{2|K_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}}|}{2^{q_++q_--N}Tr\left(\left[\pi^+_{n_1}...\pi^+_{n_{q_+}}\ \pi^-_{m_1}...\pi^-_{m_{q_-}} - \pi^-_{n_1}...\pi^-_{n_{q_+}}\ \pi^+_{m_1}...\pi^+_{m_{q_-}}\right] H_{diag}\right)} \tag{114}$$

where the denominator only involves the $z-$couplings concerning the spins n_α, m_β.

As an example, the XXZ chain with random fields of Eq. 20 contains initially off-diagonal terms of the form

$$J_i(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) = K_{0;i;i+1}(l)\left(X^\dagger_{0;i,i+1} + X_{0;i,i+1}\right) \tag{115}$$

This given term can be suppressed via the unitary transformation with $\phi = 0$

$$\begin{aligned} u = e^{\eta} &= e^{\theta(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+)} \\ &= 1 + (\cos\theta - 1)(\pi_i^+\pi_{i+1}^- + \pi_i^-\pi_{i+1}^+) + \sin\theta(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+) \\ &= 1 + (\cos\theta - 1)\frac{1-\sigma_i^z\sigma_{i+1}^z}{2} + \sin\theta(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+) \end{aligned} \tag{116}$$

where the angle θ has to be chosen as (Eq. 114)

$$\begin{aligned} \tan(2\theta) &= \frac{2J_i}{2^{2-N}Tr\left(\left[\pi_i^+\pi_{i+1}^- - \pi_i^-\pi_{i+1}^+\right] H_{diag}\right)} = \frac{J_i}{2^{-N}Tr\left((\sigma_i^z - \sigma_{i+1}^z)H_{diag}\right)} \\ &= \frac{J_i}{h_i - h_{i+1}} \end{aligned} \tag{117}$$

As in the Jacobi algorithm, this method tends to generate all possible off-diagonal couplings in the running Hamiltonian of Eq. 106 even if one starts from a sparse initial condition, so that one needs to introduce some truncations in the numerical application of this procedure : we refer to References [4, 5] for discussions and examples of numerical results that can be obtained.

VI. CONTINUOUS FRAMEWORK FOR QUANTUM SPIN HAMILTONIANS

In the continuous framework, the most general anti-hermitian generator can be expanded in terms of all the operators involved in the off-diagonal part of Eq. 106

$$\eta(l) = \sum_{q_+=1}^{N}\sum_{q_-=0}^{N-q_+}\sum_{q_z=0}^{N-q_+-q_-}\sum_{n_{(1\leq\alpha\leq q_+)}}\sum_{m_{(1\leq\beta\leq q_-)}}\sum_{p_{(1\leq\alpha\leq q_z)}}\theta_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l) \tag{118}$$

$$\left[e^{i\phi_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l)}X^\dagger_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}} - e^{-i\phi_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l)}X_{p_1,..p_{q_z};n_1,..,n_{q_+},m_1,..,m_{q_-}}\right]$$

where the generalized angles $\theta_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l)$ and $\phi_{p_1,..p_{q_z};n_1,..,n_{q_+};m_1,..,m_{q_-}}(l)$ define the choice of η.

In particular, the Wegner's choice of Eq. 55

$$\eta^{Wegner}(l) = [H_{diag}(l), H(l)] = [H_{diag}(l), H_{off}(l)] \tag{119}$$

has been applied to many different condensed matter problems (see the reviews [7], the book [8] and references therein).

The White's choice of Eq. 66

$$[\eta^{White}(l), H_{diag}(l)] = -H_{off}(l) \tag{120}$$

has been applied numerically and compared to the discrete Jacobi framework in Ref [4].

As in the Jacobi method, these Wegner's and White's flows based on the systematic decay of I_2^{off} tend to generate all possible off-diagonal couplings in the running Hamiltonian of Eq. 106, and one has again to introduce some truncation in the numerical implementation.

VII. ADAPTATION OF THE IDEA OF THE TODA FLOW TO QUANTUM SPIN CHAINS

A. Ansatz for a simplified closed flow

Let us now focus on the XXZ chain of Eq. 20 as the initial state. We would like to define the 'best closed flow' of the form

$$H^{XXZ}(l) \quad = H_{diag}\{\sigma_r^z\} + \sum_n \mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\}(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+) \tag{121}$$

where the diagonal part is written as $H_{diag}\{\sigma_r^z\}$ to emphasize that it depends on the N operators σ_r^z via the expansion involving 2^N real running coefficients $H_{a_1...a_N}(l)$

$$H_{diag}\{\sigma_r^z\} = \sum_{a_1=0,z} ... \sum_{a_N=0,z} H_{a_1...a_N}(l)\sigma_1^{(a_1)}\sigma_2^{(a_2)}...\sigma_N^{(a_N)} \tag{122}$$

as in the final state at $l=\infty$ of Eq. 26. Similarly, the prefactor of the elementary off-diagonal operator $(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)$ in Eq. 121 is written as $\mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\}$ to emphasize that it depends on the $(N-2)$ operators $\sigma^z_{r\neq(n,n+1)}$ via the expansion involving 2^{N-2} real running coefficients $J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l)$

$$\mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\} = \sum_{a_1=0,z} ... \sum_{a_{n-1}=0,z} \sum_{a_{n+2}=0,z} ... \sum_{a_N=0,z} J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l)\sigma_1^{(a_1)}...\sigma_{n-1}^{(a_{n-1})}\sigma_{n+2}^{(a_{n+2})}...\sigma_N^{(a_N)} \tag{123}$$

So the simplification with respect to the most general off-diagonal Hamiltonian of Eq. 106 is that only terms corresponding to the operators $X_{0,n,n+1} = \sigma_n^+\sigma_{n+1}^-$ are included.

Accordingly, the generator is chosen to include only the off-diagonal operators $X_{0,n,n+1} = \sigma_n^+\sigma_{n+1}^-$ (instead of the most general form of Eq. 118)

$$\eta \quad = \sum_i \Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+) \tag{124}$$

where $\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}$ depends on the $(N-2)$ operators $\sigma^z_{k\neq(i,i+1)}$ via the expansion involving 2^{N-2} real running coefficients $\theta_i(a_1,..,a_{i-1},a_{i+2}..,a_N;l)$

$$\Theta_i\{\sigma^z_{r\neq(i,i+1)}\} = \sum_{a_1=0,z} ... \sum_{a_{i-1}=0,z} \sum_{a_{i+1}=0,z} ... \sum_{a_N=0,z} \theta_i(a_1,..,a_{i-1},a_{i+2}..,a_N;l)\sigma_1^{(a_1)}...\sigma_{i-1}^{(a_{i-1})}\sigma_{i+2}^{(a_{i+2})}...\sigma_N^{(a_N)} \tag{125}$$

Our goal is to choose the generator η to maintain the flow of the Hamiltonian of Eq. 121 as 'closed' as possible.

B. Flow equation

With the above Ansatz, the flow equation reads

$$\begin{aligned}
\frac{dH}{dl} = [\eta, H] \quad &= \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), H_{diag}\{\sigma_r^z\}] \\
&+ \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \mathcal{J}_i\{\sigma^z_{r\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+)] \\
&+ \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \mathcal{J}_{i-1}\{\sigma^z_{r\neq(i-1,i)}\}(\sigma_{i-1}^+\sigma_i^- + \sigma_{i-1}^-\sigma_i^+)] \\
&+ \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \mathcal{J}_{i+1}\{\sigma^z_{r\neq(i+1,i+2)}\}(\sigma_{i+1}^+\sigma_{i+2}^- + \sigma_{i+1}^-\sigma_{i+2}^+)] \\
&+ \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \sum_{n\neq(i-1,i,i+1)} \mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\}(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)]
\end{aligned} \tag{126}$$

To compute these various commutators, it is useful to introduce for any function $f\{\sigma_r^z\}$ its expansion with respect to a given spin σ_i^z

$$f\{\sigma_r^z\} \quad = f^{(i,0)}\{\sigma^z_{r\neq i}\} + \sigma_i^z f^{(i,1)}\{\sigma^z_{r\neq i}\} \tag{127}$$

where the two auxiliary functions can be obtained by some traces with respect to the single spin σ_i

$$\begin{aligned} f^{(i,0)}\{\sigma^z_{r\neq i}\} &= \frac{1}{2} Tr_{\sigma_i}(f\{\sigma^z_r\}) \\ f^{(i,1)}\{\sigma^z_{r\neq i}\} &= \frac{1}{2} Tr_{\sigma_i}(\sigma^z_i f\{\sigma^z_r\}) \end{aligned} \tag{128}$$

Similarly, its expansion with respect to a pair of given spins (σ^z_i, σ^z_j) reads

$$f\{\sigma^z_r\} = f^{(i,0)(j,0)}\{\sigma^z_{r\neq i,j}\} + \sigma^z_i f^{(i,1)(j,0)}\{\sigma^z_{r\neq i,j}\} + \sigma^z_j f^{(i,0)(j,1)}\{\sigma^z_{r\neq i,j}\} + \sigma^z_i \sigma^z_j f^{(i,1)(j,1)}\{\sigma^z_{r\neq i,j}\} \tag{129}$$

where the four auxiliary functions can be obtained by some traces with respect to the two spins (σ_i, σ_j)

$$\begin{aligned} f^{(i,0)(j,0)}\{\sigma^z_{r\neq i,j}\} &= \frac{1}{2^2} Tr_{\sigma_i,\sigma_j}(f\{\sigma^z_r\}) \\ f^{(i,1)(j,0)}\{\sigma^z_{r\neq i,j}\} &= \frac{1}{2^2} Tr_{\sigma_i,\sigma_j}(\sigma^z_i f\{\sigma^z_r\}) \\ f^{(i,0)(j,1)}\{\sigma^z_{r\neq i,j}\} &= \frac{1}{2^2} Tr_{\sigma_i,\sigma_j}(\sigma^z_j f\{\sigma^z_r\}) \\ f^{(i,1)(j,1)}\{\sigma^z_{r\neq i,j}\} &= \frac{1}{2^2} Tr_{\sigma_i,\sigma_j}(\sigma^z_i \sigma^z_j f\{\sigma^z_r\}) \end{aligned} \tag{130}$$

Using the expansion of Eq. 129 for the diagonal Hamiltonian

$$\begin{aligned} H_{diag}\{\sigma^z_r\} &= H^{(i,0)(i+1,0)}_{diag}\{\sigma^z_{r\neq i,i+1}\} + \sigma^z_i H^{(i,1)(i+1,0)}_{diag}\{\sigma^z_{r\neq i,i+1}\} + \sigma^z_{i+1} H^{(i,0)(i+1,1)}_{diag}\{\sigma^z_{r\neq i,i+1}\} \\ &+ \sigma^z_i \sigma^z_{i+1} H^{(i,1)(i+1,1)}_{diag}\{\sigma^z_{r\neq i,i+1}\} \end{aligned} \tag{131}$$

the first line of the flow Eq. 126 becomes

$$\left(\frac{dH}{dl}\right)_{first} = 2\sum_i \Theta_i\{\sigma^z_{k\neq(i,i+1)}\}\left(H^{(i,0)(i+1,1)}_{diag}\{\sigma^z_{r\neq i,i+1}\} - H^{(i,1)(i+1,0)}_{diag}\{\sigma^z_{r\neq i,i+1}\}\right)(\sigma^+_i \sigma^-_{i+1} + \sigma^-_i \sigma^+_{i+1}) \tag{132}$$

It is thus compatible with the flow Ansatz of Eq. 121 and will actually be the only contribution to the flow of the $\mathcal{J}_i\{\sigma^z_{r\neq(n,n+1)}\}$ that reads

$$\frac{d\mathcal{J}_i\{\sigma^z_{r\neq(i,i+1)}\}}{dl} = 2\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}\left(H^{(i,0)(i+1,1)}_{diag}\{\sigma^z_{r\neq i,i+1}\} - H^{(i,1)(i+1,0)}_{diag}\{\sigma^z_{r\neq i,i+1}\}\right) \tag{133}$$

The second line of Eq. 126

$$\begin{aligned} \left(\frac{dH}{dl}\right)_{second} &\equiv \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma^+_i \sigma^-_{i+1} - \sigma^-_i \sigma^+_{i+1}), \mathcal{J}_i\{\sigma^z_{r\neq(i,i+1)}\}(\sigma^+_i \sigma^-_{i+1} + \sigma^-_i \sigma^+_{i+1})] \\ &= \sum_i \Theta_i\{\sigma^z_{k\neq(i,i+1)}\}\mathcal{J}_i\{\sigma^z_{r\neq(i,i+1)}\}(\sigma^z_i - \sigma^z_{i+1}) \end{aligned} \tag{134}$$

is also compatible with the flow Ansatz of Eq. 121 and will actually be the only contribution to the flow of the diagonal part that reads

$$\frac{dH_{diag}\{\sigma^z_r\}}{dl} = \sum_i \Theta_i\{\sigma^z_{k\neq(i,i+1)}\}\mathcal{J}_i\{\sigma^z_{r\neq(i,i+1)}\}(\sigma^z_i - \sigma^z_{i+1}) \tag{135}$$

Using the notations of Eq. 127, the third and the fourth lines of Eq. 126 lead to the global result

$$\begin{aligned}
\left(\frac{dH}{dl}\right)_{third} + \left(\frac{dH}{dl}\right)_{fourth} &\equiv \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \mathcal{J}_{i-1}\{\sigma^z_{r\neq(i-1,i)}\}(\sigma_{i-1}^+\sigma_i^- + \sigma_{i-1}^-\sigma_i^+)] \\
&+ \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \mathcal{J}_{i+1}\{\sigma^z_{r\neq(i+1,i+2)}\}(\sigma_{i+1}^+\sigma_{i+2}^- + \sigma_{i+1}^-\sigma_{i+2}^+)] \\
= \sum_i (\Theta_i^{(i-1,0)}&\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_{i-1}^{(i+1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} + \Theta_i^{(i-1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_{i-1}^{(i+1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} \\
-\mathcal{J}_i^{(i-1,0)}&\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_{i-1}^{(i+1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} - \mathcal{J}_i^{(i-1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_{i-1}^{(i+1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}) \\
(\sigma_{i-1}^+\sigma_i^z&\sigma_{i+1}^- + \sigma_{i-1}^-\sigma_i^z\sigma_{i+1}^+) \\
+\sum_i (\mathcal{J}_{i-1}^{(i+1,0)}&\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_i^{(i-1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} + \mathcal{J}_{i-1}^{(i+1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_i^{(i-1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} \\
-\Theta_{i-1}^{(i+1,0)}&\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_i^{(i-1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} - \Theta_{i-1}^{(i+1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_i^{(i-1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}) \\
(\sigma_{i-1}^+\sigma_{i+1}^-& + \sigma_{i-1}^-\sigma_{i+1}^+)
\end{aligned} \tag{136}$$

So these terms tend to generate off-diagonal terms containing two ladder operators concerning two spins at distance two of the form $(\sigma_{i-1}^+\sigma_{i+1}^- + \sigma_{i-1}^-\sigma_{i+1}^+)$ that are not present in the Ansatz of Eq. 121 : to avoid the creation of these new terms, one can require that the prefactors containing σ^z operators identically vanish and one obtains the constraints

$$\begin{aligned}
&\Theta_i^{(i-1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_{i-1}^{(i+1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} + \Theta_i^{(i-1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_{i-1}^{(i+1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} \\
&= \mathcal{J}_i^{(i-1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_{i-1}^{(i+1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} + \mathcal{J}_i^{(i-1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_{i-1}^{(i+1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\})
\end{aligned} \tag{137}$$

and

$$\begin{aligned}
&\mathcal{J}_{i-1}^{(i+1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_i^{(i-1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} + \mathcal{J}_{i-1}^{(i+1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}\Theta_i^{(i-1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\} \\
&= \Theta_{i-1}^{(i+1,0)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_i^{(i-1,1)}\{\sigma^z_{r\neq(i-1,i,i+1)}\} + \Theta_{i-1}^{(i+1,1)}\{\sigma^z_{k\neq(i-1,i,i+1)}\}\mathcal{J}_i^{(i-1,0)}\{\sigma^z_{r\neq(i-1,i,i+1)}\}
\end{aligned} \tag{138}$$

It is clear that a simple solution for the functions $\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}$ defining the generator η is the choice that generalizes the Toda case of Eq 84

$$\Theta_i^{Toda}\{\sigma^z_{k\neq(i,i+1)}\} = \mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\} \tag{139}$$

Then the contribution of Eq. 136 vanish

$$\left(\frac{dH}{dl}\right)^{Toda}_{third} + \left(\frac{dH}{dl}\right)^{Toda}_{fourth} = 0 \tag{140}$$

Finally, using the notations of Eq. 129, the fifth and last line of Eq. 126

$$\begin{aligned}
\left(\frac{dH}{dl}\right)_{fifth} &\equiv \sum_i [\Theta_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \sum_{n\neq(i-1,i,i+1)} \mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\}(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)] \\
= 2\sum_i \sum_{n\neq(i-1,i,i+1)} &\left(\Theta_i^{(n,0)(n+1,0)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\} - \Theta_i^{(n,1)(n+1,1)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\}\right) \\
\left(\mathcal{J}_n^{(i,0)(i+1,1)}\right.&\left.\{\sigma^z_{r\neq(i,i+1,n,n+1)}\} - \mathcal{J}_n^{(i,1)(i+1,0)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\}\right)(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+)(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+) \\
+2\sum_i \sum_{n\neq(i-1,i,i+1)} &\left(\Theta_i^{(n,1)(n+1,0)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\} - \Theta_i^{(n,0)(n+1,1)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\}\right) \\
\left(\mathcal{J}_n^{(i,0)(i+1,0)}\right.&\left.\{\sigma^z_{r\neq(i,i+1,n,n+1)}\} - \mathcal{J}_n^{(i,1)(i+1,1)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\}\right)(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+)(\sigma_n^+\sigma_{n+1}^- - \sigma_n^-\sigma_{n+1}^+)
\end{aligned} \tag{141}$$

tends to generate off-diagonal terms containing four ladder operators concerning two pairs of consecutive spins $(i, i+1)$

and $(n,n+1)$ that are not present in the Ansatz of Eq. 121. With the choice of Eq. 139, Eq. 141 can be reduced to

$$\left(\frac{dH}{dl}\right)_{fifth}$$
$$= 4\sum_i \sum_{n\neq(i-1,i,i+1)} \left(\mathcal{J}_i^{(n,0)(n+1,0)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\} - \mathcal{J}_i^{(n,1)(n+1,1)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\}\right)$$
$$\left(\mathcal{J}_n^{(i,0)(i+1,1)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\} - \mathcal{J}_n^{(i,1)(i+1,0)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\}\right)(\sigma_i^+\sigma_{i+1}^-\sigma_n^-\sigma_{n+1}^+ + \sigma_i^-\sigma_{i+1}^+\sigma_n^+\sigma_{n+1}^-) \quad (142)$$

C. Definition of the analog of the Toda flow

In summary, we have explained in the previous section that the choice of Eq. 139

$$\Theta_i^{Toda}\{\sigma^z_{k\neq(i,i+1)}\} = \mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\} \quad (143)$$

for the generator of Eq. 84 corresponds to the best approximation of a closed flow for the running Hamiltonian of Eq. 121 because it suppresses the generation of the most important new off-diagonal containing two ladder operators concerning non-consecutive spins. The only non-closed term involves four ladder operators (Eq. 142)

$$\left(\frac{dH}{dl}\right)_{non-closed} = 4\sum_i \sum_{n\neq(i-1,i,i+1)} \left(\mathcal{J}_i^{(n,0)(n+1,0)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\} - \mathcal{J}_i^{(n,1)(n+1,1)}\{\sigma^z_{k\neq(i,i+1,n,n+1)}\}\right)$$
$$\left(\mathcal{J}_n^{(i,0)(i+1,1)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\} - \mathcal{J}_n^{(i,1)(i+1,0)}\{\sigma^z_{r\neq(i,i+1,n,n+1)}\}\right)(\sigma_i^+\sigma_{i+1}^-\sigma_n^-\sigma_{n+1}^+ + \sigma_i^-\sigma_{i+1}^+\sigma_n^+\sigma_{n+1}^-) \quad (144)$$

With the choice of Eq. 143, the coupled flow equations for the diagonal part $H_{diag}\{\sigma_k^z\}$ and for the generalized couplings $\mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\}$ of Eqs 133 and 135 become

$$\frac{dH_{diag}\{\sigma_k^z\}}{dl} = \sum_i \mathcal{J}_i^2\{\sigma^z_{r\neq(i,i+1)}\}(\sigma_i^z - \sigma_{i+1}^z) \quad (145)$$

and

$$\frac{d\mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\}}{dl} = 2\mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\}\left(H_{diag}^{(i,0)(i+1,1)}\{\sigma^z_{r\neq i,i+1}\} - H_{diag}^{(i,1)(i+1,0)}\{\sigma^z_{r\neq i,i+1}\}\right) \quad (146)$$

with the notations of Eq. 130 and Eq. 122

$$\begin{aligned}
H_{diag}^{(i,1)(i+1,0)}\{\sigma^z_{r\neq i,i+1}\} &= \frac{1}{2^2}Tr_{\sigma_i,\sigma_i+1}(\sigma_i^z H_{diag}\{\sigma_r^z\}) \\
&= \sum_{a_1=0,z}... \sum_{a_{i-1}=0,z}\sum_{a_{i+2}=0,z}...\sum_{a_N=0,z} H_{a_1,..,a_{i-1},a_i=1,a_{i+1}=0,a_{i+2}...a_N}(l)\sigma_1^{(a_1)}...\sigma_{i-1}^{(a_{i-1})}\sigma_{i+2}^{(a_{i+2})}...\sigma_N^{(a_N)} \\
H_{diag}^{(i,0)(i+1,1)}\{\sigma^z_{r\neq i,i+1}\} &= \frac{1}{2^2}Tr_{\sigma_i,\sigma_i+1}(\sigma_{i+1}^z H_{diag}\{\sigma_r^z\}) \\
&= \sum_{a_1=0,z}... \sum_{a_{i-1}=0,z}\sum_{a_{i+2}=0,z}...\sum_{a_N=0,z} H_{a_1,..,a_{i-1},a_i=0,a_{i+1}=1,a_{i+2}...a_N}(l)\sigma_1^{(a_1)}...\sigma_{i-1}^{(a_{i-1})}\sigma_{i+2}^{(a_{i+2})}...\sigma_N^{(a_N)}
\end{aligned} \quad (147)$$

D. Conservation of the invariant I_2 by the flow

Since we have made the approximation that one could neglect the terms of Eq. 144, it is important to consider the dynamics of the exact invariant I_2 via the approximated closed flow of Eqs 145 and 146.

For the Hamiltonian of Eq. 121, one obtains

$$\begin{aligned}
I_2(l) &\equiv \frac{1}{2^N}Tr(H^2(l)) = \frac{1}{2^N}Tr\left(H_{diag}\{\sigma_r^z\} + \sum_n \mathcal{J}_n\{\sigma^z_{r\neq(n,n+1)}\}(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)\right)^2 \\
&= \frac{1}{2^N}Tr\left(H_{diag}^2(\sigma_r^z) + \sum_n \frac{\mathcal{J}_n^2(\sigma_r^z)}{2}\right)
\end{aligned} \quad (148)$$

Using Eq. 145, the diagonal contribution evolves according to

$$I_2^{diag}(l) = \frac{1}{2^N} Tr \left(H^2_{diag}(\sigma^z_r) \right) \tag{149}$$

evolves according to

$$\frac{dI_2^{diag}(l)}{dl} = \frac{2}{2^N} Tr \left(\frac{dH_{diag}(\sigma^z_r)}{dl} H_{diag}(\sigma^z_r) \right) = \frac{2}{2^N} \sum_i Tr \left(\mathcal{J}_i^2 \{\sigma^z_{r \neq (i,i+1)}\} (\sigma^z_i - \sigma^z_{i+1}) H_{diag}(\sigma^z_r) \right) \tag{150}$$

Since the $\mathcal{J}_i^2 \{\sigma^z_{r \neq (i,i+1)}\}$ does not depend on the two spins σ_i and σ_{i+1}, the partial trace over these two spins alone can be evaluated with the expansion of $H_{diag}(\sigma^z_r)$ of Eq. 131 yielding

$$\begin{aligned}
Tr_{\sigma_i,\sigma_{i+1}} \left((\sigma^z_i - \sigma^z_{i+1}) H_{diag}(\sigma^z_r) \right) &= Tr_{\sigma_i,\sigma_{i+1}} \left((\sigma^z_i H_{diag}(\sigma^z_r) - \sigma^z_{i+1} H_{diag}(\sigma^z_r) \right) \\
&= 4 H^{(i,1)(i+1,0)}_{diag} \{\sigma^z_{r \neq i,i+1}\} - 4 H^{(i,0)(i+1,1)}_{diag} \{\sigma^z_{r \neq i,i+1}\} \\
&= Tr_{\sigma_i,\sigma_{i+1}} \left(H^{(i,1)(i+1,0)}_{diag} \{\sigma^z_{r \neq i,i+1}\} - H^{(i,0)(i+1,1)}_{diag} \{\sigma^z_{r \neq i,i+1}\} \right)
\end{aligned} \tag{151}$$

so that Eq. 150 can be rewritten as

$$\frac{dI_2^{diag}(l)}{dl} = \frac{2}{2^N} \sum_i Tr \left(\mathcal{J}_i^2 \{\sigma^z_{r \neq (i,i+1)}\} \left(H^{(i,1)(i+1,0)}_{diag} \{\sigma^z_{r \neq i,i+1}\} - H^{(i,0)(i+1,1)}_{diag} \{\sigma^z_{r \neq i,i+1}\} \right) \right) \tag{152}$$

On the other hand, using Eq. 146, the off-diagonal contribution in Eq. 148

$$I_2^{off}(l) = \frac{1}{2^N} \sum_n Tr \left(\frac{\mathcal{J}_i^2(\sigma^z_r)}{2} \right) \tag{153}$$

evolves according to

$$\begin{aligned}
\frac{dI_2^{off}(l)}{dl} &= \frac{1}{2^N} \sum_n Tr \left(\mathcal{J}_i(\sigma^z_r) \frac{d\mathcal{J}_i \{\sigma^z_{k \neq (i,i+1)}\}}{dl} \right) \\
&= \frac{2}{2^N} \sum_n Tr \left(\mathcal{J}_i^2(\sigma^z_r) \left(H^{(i,0)(i+1,1)}_{diag} \{\sigma^z_{r \neq i,i+1}\} - H^{(i,1)(i+1,0)}_{diag} \{\sigma^z_{r \neq i,i+1}\} \right) \right)
\end{aligned} \tag{154}$$

so that the sum with Eq. 152 yields the conservation of $I_2(l)$ of Eq. 148

$$\frac{dI_2(l)}{dl} = \frac{dI_2^{diag}(l)}{dl} + \frac{dI_2^{off}(l)}{dl} = 0 \tag{155}$$

E. Exactness of the flow for the random XX chain with random fields

When the initial model is the random XX chain with random fields $J^{zz}_n = 0$, one obtains that the Ansatz of Eq. 121 is an exact solution of the flow

$$H^{XX}(l) = H^{XX}_{diag} \{\sigma^z_r\} + \sum_n \mathcal{J}^{XX}_n \{\sigma^z_{r \neq (n,n+1)}\} (\sigma^+_n \sigma^-_{n+1} + \sigma^-_n \sigma^+_{n+1}) \tag{156}$$

where the diagonal part reduces to running random fields $h_i(l)$

$$H^{XX}_{diag}(\{\sigma^z_r\}) = \sum_{i=1}^N h_i(l) \sigma^z_i \tag{157}$$

while $\mathcal{J}^{XX}_n \{\sigma^z_{r \neq (n,n+1)}\}$ reduce to running couplings $J_n(l)$

$$\mathcal{J}^{XX}_n \{\sigma^z_{r \neq (n,n+1)}\} = J_n(l) \tag{158}$$

so that the generation of terms with four operators in Eq. 144 identically vanishes

$$\left(\frac{dH}{dl} \right)_{non-closed} = 0 \tag{159}$$

The coupled flow Equations 145 and 146 reduce to

$$\frac{dh_i(l)}{dl} = J_i^2 - J_{i-1}^2 \tag{160}$$

and

$$\frac{dJ_i(l)}{dl} = 2J_i(l) \left(h_{i+1}(l) - h_i(l) \right) \tag{161}$$

so that they coincide with the Toda flow for tridiagonal matrices of Eq. 87 via the identification $H_{i,i+1} = J_i$ and $H_{i,i} = 2h_i$. This equivalence is consistent with the tridiagonal matrix in the fermion language of Eq. 24 that has to be diagonalized to obtain the free-fermions eigenvalues. So here the Toda flow leads directly to the diagonal final result of Eq. 25 within the spin language, without going through the explicit Jordan-Wigner transformation onto free-fermions operators (Eq 23).

F. Flow Equations for the real coefficients

Using the expansion of Eq. 123, one obtains the expansion of the square

$$\begin{aligned} \mathcal{J}_n^2\{\sigma^z_{r\neq(n,n+1)}\} &= \sum_{a_1=0,z} ... \sum_{a_{n-1}=0,z} \sum_{a_{n+2}=0,z} ... \sum_{a_N=0,z} J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l) \\ & \sum_{b_1=0,z} ... \sum_{b_{n-1}=0,z} \sum_{b_{n+2}=0,z} ... \sum_{b_N=0,z} J_n(b_1,..,b_{n-1},b_{n+2}..,b_N;l) \\ & (\sigma_1^{(a_1)}\sigma_1^{(b_1)})...(\sigma_{n-1}^{(a_{n-1})}\sigma_{n-1}^{(b_{n-1})})(\sigma_{n+2}^{(a_{n+2})}\sigma_{n+2}^{(b_{n+2})})...(\sigma_N^{(a_N)}\sigma_N^{(b_N)}) \end{aligned} \tag{162}$$

so that the flow Equation 145 becomes

$$\begin{aligned} \frac{dH_{diag}\{\sigma_k^z\}}{dl} &= \sum_n \mathcal{J}_n^2\{\sigma^z_{r\neq(n,n+1)}\}(\sigma_n^z - \sigma_{n+1}^z) \\ &= \sum_n \sum_{a_1=0,z} ... \sum_{a_{n-1}=0,z} \sum_{a_{n+2}=0,z} ... \sum_{a_N=0,z} J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l) \\ & \sum_{b_1=0,z} ... \sum_{b_{n-1}=0,z} \sum_{b_{n+2}=0,z} ... \sum_{b_N=0,z} J_n(b_1,..,b_{n-1},b_{n+2}..,b_N;l) \\ & (\sigma_1^{(a_1)}\sigma_1^{(b_1)})...(\sigma_{n-1}^{(a_{n-1})}\sigma_{n-1}^{(b_{n-1})})(\sigma_n^z - \sigma_{n+1}^z)(\sigma_{n+2}^{(b_{n+2})})...(\sigma_N^{(a_N)}\sigma_N^{(b_N)}) \end{aligned} \tag{163}$$

Using the properties of the Pauli matrices $\sigma^{(0)} = Id$ and σ_i^z

$$\sigma_i^{(a_i)}\sigma_i^{(b_i)} = \delta_{a_i,b_i}\sigma_i^{(0)} + (1-\delta_{a_i,b_i})\sigma_i^z \tag{164}$$

this can be rewritten as flow equations for the 2^N real coefficients of the diagonal part of Eq. 122 as

$$\begin{aligned} \frac{dH_{c_1...c_N}(l)}{dl} &= \sum_n \sum_{a_1=0,z} ... \sum_{a_{n-1}=0,z} \sum_{a_{n+2}=0,z} ... \sum_{a_N=0,z} J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l) \\ & \sum_{b_1=0,z} ... \sum_{b_{n-1}=0,z} \sum_{b_{n+2}=0,z} ... \sum_{b_N=0,z} J_n(b_1,..,b_{n-1},b_{n+2}..,b_N;l) \\ & (\delta_{c_n,1}\delta_{c_{n+1},0} - \delta_{c_n,0}\delta_{c_{n+1},1}) \prod_{i\neq(n,n+1)} (\delta_{c_i,0}\delta_{a_i,b_i} + \delta_{c_i,z}(1-\delta_{a_i,b_i})) \end{aligned} \tag{165}$$

For instance the flow equations for the random fields $h_i(l)$ with only a single non-vanishing index $c_i = z$ reads

$$\frac{dh_i(l)}{dl} = \frac{dH_{c_1=0,..c_{i-1}=0,,c_i=1,c_{i+1}=0,.....c_N=0}(l)}{dl} \tag{166}$$
$$= \sum_{a_1=0,z} ... \sum_{a_{i-2}=0,z} \sum_{a_{i+2}=0,z} ... \sum_{a_N=0,z} \left(\sum_{a_{i-1}=0,z} J_i^2(a_1,..,a_{i-1},a_{i+2}..,a_N;l) - \sum_{a_{i+1}=0,z} J_{i-1}^2(a_1,..,a_{i-2},a_{i+1}..,a_N;l) \right)$$

Similarly, the flow Eq. 146 can be expanded into coefficients using Eqs 123 and 147

$$\begin{aligned}
\frac{d\mathcal{J}_n\{\sigma^z_{k\neq(n,n+1)}\}}{dl} &= 2\mathcal{J}_n\{\sigma^z_{k\neq(n,n+1)}\} \left(H_{diag}^{(n,0)(n+1,1)}\{\sigma^z_{r\neq n,n+1}\} - H_{diag}^{(n,1)(n+1,0)}\{\sigma^z_{r\neq n,n+1}\} \right) \\
&= 2 \sum_{a_1=0,z} ... \sum_{a_{i-1}=0,z} \sum_{a_{i+2}=0,z} ... \sum_{a_N=0,z} H_{a_1,..,..a_N}(l)(\delta_{a_n,0}\delta_{a_{n+1},1} - \delta_{a_n,1}\delta_{a_{n+1},0}) \\
&\sum_{b_1=0,z} ... \sum_{b_{n-1}=0,z} \sum_{b_{n+2}=0,z} ... \sum_{b_N=0,z} J_n(b_1,..,b_{n-1},b_{n+2}..,b_N;l) \\
&(\sigma_1^{(a_1)}\sigma_1^{(b_1)})...(\sigma_{n-1}^{(a_{n-1})}\sigma_{n-1}^{(b_{n-1})})(\sigma_{n+2}^{(a_{n+2})}\sigma_{n+2}^{(b_{n+2})})...(\sigma_N^{(a_N)}\sigma_N^{(b_N)})
\end{aligned} \tag{167}$$

Using again Eq. 164 this can be rewritten as flow equations for the real coefficients of Eq. 123 as

$$\begin{aligned}
\frac{dJ_n(c_1,..,c_{n-1},c_{n+2}..,c_N;l)}{dl} &= 2 \sum_{a_1=0,z} ... \sum_{a_{i-1}=0,z} \sum_{a_{i+2}=0,z} ... \sum_{a_N=0,z} H_{a_1,..,..a_N}(l)(\delta_{a_n,0}\delta_{a_{n+1},1} - \delta_{a_n,1}\delta_{a_{n+1},0}) \\
&\sum_{b_1=0,z} ... \sum_{b_{n-1}=0,z} \sum_{b_{n+2}=0,z} ... \sum_{b_N=0,z} J_n(b_1,..,b_{n-1},b_{n+2}..,b_N;l) \\
&\prod_{i\neq(n,n+1)} (\delta_{c_i,0}\delta_{a_i,b_i} + \delta_{c_i,z}(1-\delta_{a_i,b_i}))
\end{aligned} \tag{168}$$

For instance the flow equations for the $J_n(l)$ where all indices vanish $c_i = 0$ reads

$$\frac{dJ_n(l)}{dl} = \frac{dJ_n(c_1=0,..,c_{n-1}=0,c_{n+2}=0..,c_N=0;l)}{dl} \tag{169}$$
$$= 2 \sum_{a_1=0,z} ... \sum_{a_{i-1}=0,z} \sum_{a_{i+2}=0,z} ... \sum_{a_N=0,z} H_{a_1,..,..a_N}(l)(\delta_{a_n,0}\delta_{a_{n+1},1} - \delta_{a_n,1}\delta_{a_{n+1},0}) J_n(a_1,..,a_{n-1},a_{n+2}..,a_N;l)$$

We thus hope that the flow Equations 165 and 168 for the real coefficients can be used to study various truncations in the number of non-vanishing indices for the most relevant couplings, and can be studied to higher orders than in the discrete scheme [5].

G. Transformation of the spin operators

Up to now we have focused only on the flow of the Hamiltonian, but it is of course interesting to consider the flow of other observables A via the flow equation analogous to Eq. 47

$$\frac{dA(l)}{dl} = [\eta(l), A(l)] \tag{170}$$

With the choice of the Toda generator of Eq. 143, the creation operators evolve according to

$$\begin{aligned}
\frac{d\sigma_n^+}{dl} = [\eta(l), \sigma_n^+] &= \sum_i [\mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+), \sigma_n^+] \\
&= \left(\mathcal{J}_n\{\sigma^z_{k\neq(n,n+1)}\}\sigma_n^z \right) \sigma_{n+1}^+ - \left(\mathcal{J}_{n-1}\{\sigma^z_{k\neq(n-1,n)}\}\sigma_n^z \right) \sigma_{n-1}^+ \\
&+2 \sum_{i\neq(n-1,n)} \mathcal{J}_i^{(n,1)}\{\sigma^z_{k\neq(i,i+1)}\}\sigma_n^+(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+)
\end{aligned} \tag{171}$$

The annihilation operators evolve similarly as

$$\begin{aligned}\frac{d\sigma_n^-}{dl} &= \left(\mathcal{J}_n\{\sigma^z_{k\neq(n,n+1)}\}\sigma_n^z\right)\sigma^-_{n+1} - \left(\mathcal{J}_{n-1}\{\sigma^z_{k\neq(n-1,n)}\}\sigma_n^z\right)\sigma^-_{n-1} \\ &-2\sum_{i\neq(n-1,n)} \mathcal{J}_i^{(n,1)}\{\sigma^z_{k\neq(i,i+1)}\}\sigma_n^-(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+)\end{aligned} \tag{172}$$

while the operators σ_n^z evolve as

$$\begin{aligned}\frac{d\sigma_n^z}{dl} &= [\eta,\sigma_n^z] = \sum_i [\mathcal{J}_i\{\sigma^z_{k\neq(i,i+1)}\}(\sigma_i^+\sigma_{i+1}^- - \sigma_i^-\sigma_{i+1}^+),\sigma_n^z] \\ &= 2\mathcal{J}_{n-1}\{\sigma^z_{k\neq(n-1,n-1+1)}\}(\sigma^+_{n-1}\sigma_n^- + \sigma^-_{n-1}\sigma_n^+) - 2\mathcal{J}_n\{\sigma^z_{k\neq(n,n+1)}\}(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)\end{aligned} \tag{173}$$

VIII. CONCLUSION

In this paper, we have revisited the various flows towards diagonalization that have been introduced in the past, in order to stress the freedom in the choices that can be made :
(i) discrete or continuous formulation
(ii) strategy based on the steady decay of I_2^{off} or on the repeated application of the Hamiltonian
(iii) schemes that tend to generate all possible couplings in the running Hamiltonian or schemes that are able to preserve some 'sparsity' of the initial condition.

We have then focused on the random XXZ chain with random fields in order to determine the best closed flow within the subspace of running Hamiltonians containing only two ladder operators on consecutive sites. For the special case of the free-fermion random XX chain with random fields, we have shown that the flow coincides with the Toda differential flow for tridiagonal matrices which can be seen as the continuous analog of the discrete QR-algorithm. For the random XXZ chain with random fields that displays a Many-Body-Localization transition, the present differential flow is an interesting alternative to the discrete flow that has been proposed recently to study the Many-Body-Localization properties in a model of interacting fermions [5]. We hope that the differential flow for the XXZ-chain can be transformed into an efficient numerical procedure where the effects of the order of truncation can be systematically studied up to higher orders. Finally, since the necessity to diagonalize matrices and operators appears almost everywhere in sciences, we hope that the idea of the Toda flow can be adapted in various fields.

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